

CENTRAL UNIVERSITY OF PUNJAB, BATHINDA



**M.Sc. in Chemical Sciences
(Medicinal Chemistry)**

Session- 2019-2021

**Department of Pharmaceutical Sciences and
Natural Products**

Programme Outcome

1. Students will have enhanced academic knowledge and ability, and increased theoretical and methodological qualifications in the field of medicinal chemistry.
2. The programme will enable the students to identify and solve complex problems in organic chemistry and medicinal chemistry independently and at an academic level
3. Students will be able to explain and reflect upon the key principles used for the rational basis of design, syntheses and development of new drugs
4. Students will be able to identify scientific problems in relation to the design, syntheses and development of drugs.
5. Students will use and critically evaluate results achieved by modern computer-based methods for structural-activity analyses of biologically active compounds
6. The programme will develop research aptitude in the students with training in scientific work and methods required for a PhD degree or other research programme,
7. Students completing this programme will be competitive enough to work in the pharmaceutical or biotechnological industries in particular
8. The programme will enable to convey theoretical and research-based knowledge and communicate at a high academic level with peers, undergraduate students and non-specialists in the field of organic synthesis for drug research, computational and structural drug design.

IQAC

SEMESTER 1

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1	CST.501	Computer Applications	CF	2	-	-	2
2	CMC.506	Organic Chemistry-I	C	4	-	-	4
3	CMC.507	Organic Synthesis-I (Practical)	C	-	-	4	2
4	CMC.508	Modern Spectral and Chromatography Techniques	C	4	-	-	4
5	CMC.509	Spectral Analysis (Practical)	C	-	-	4	2
6	CMC.510	Medicinal Chemistry-I	C	3	1	-	4
7	XXX	Inter-Disciplinary (IDC) Course (Opt any one from other Departments)	ID	2	-	-	2
Opt any one course from following elective							
8	CMC.511	Chemistry of Natural Products	DE	4	-	-	4
9	CMC.512	Quantum Chemistry					
Total				19	1	8	24

CF: Compulsory Foundation, **C:** Core, **ID:** Interdisciplinary, **DE:** Discipline elective

L: Lectures T: Tutorial P: Practical Cr: Credits

Criteria of evaluation for Theory:

A: Continuous Assessment: [25 Marks]

(i). Surprise Tests (minimum three)-Based on Objective Type Tests (10 marks)

(ii). Term paper (10 marks)

(iii). Assignments (5 marks).

B: Mid-Semester Test – I: Based on Subjective Type Test [25 Marks]

C: Mid-Semester Test – II: Based on Subjective Type Test [25 Marks]

D: End-Term Exam (Final): Online Objective Type Test [25 Marks]

E: Total Marks

Evaluation criteria for Practical:

Item	Synopsis	Experiment	Practical Note book and day to day evaluation	Viva voce
Marks	10	10	20	10

6SEMESTER II

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1	CMC.521	Organic Chemistry-II	C	4	-	-	4
2	CMC.522	Organic Synthesis-II-(Practical)	C	-	-	4	2
3	CMC.523	Basics of Drug Design and Drug Action	C	3	1	-	4
4	CMC.524	Computer Aided Drug Design-(Practical)	C	-	-	4	2
5	CMC.525	Advanced Spectral Analysis	C	4	-	-	4
6	CMC.542	Seminar	SB	-	-	-	1
7	XXX	Inter-Disciplinary Course (ID) (Opt any one from other Department)	ID	2	-	-	2
8	XXX (To be decided at University level)	Value added elective course	EF	1	-	-	1
		Total		14	1	8	20

CF: Compulsory Foundation, **C:** Core, **ID:** Interdisciplinary, **DE:** Discipline elective

Criteria of evaluation for theory:

A: Continuous Assessment: [25 Marks]

(i). Surprise Tests (minimum three)-Based on Objective Type Tests (10 marks)

(ii). Term paper (10 marks)

(iii). Assignments (5 marks).

B: Mid-Semester Test – I: Based on Subjective Type Test [25 Marks]

C: Mid-Semester Test – II: Based on Subjective Type Test [25 Marks]

D: End-Term Exam (Final): Online Objective Type Test [25 Marks]

E: Total Marks

Evaluation criteria for practical:

Item	Synopsis	Experiment	Practical Note book and day to day evaluation	Viva voce
Marks	10	10	20	10

SEMESTER III

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1	CMC.551	Research Methodology	CF	1	-	-	2
2	CMC.552	Organic Chemistry-III	C	4	-	-	4
3	CMC.553	Medicinal Chemistry-II	C	4	-	-	4
4	CMC.554	Organic Chemistry-III (Practical)	C	-	-	4	2
5	XXX (To be decided at University level)	Value added elective course	EF	1	-	-	1
6	CMC.543	Seminar	SB	-	-	-	1
7	CMC.599	Project	SB	-	-	-	6
Optany one course from following elective							
8	CMC.555 CMC.556 CMC.557	Current Trends in Organic Bioinorganic and Biophysical Chemistry Nuclear Chemistry	DE	3	1	-	4
Total				13	1	4	24

CF: Compulsory Foundation, **C:** Core, **ID:** Interdisciplinary, **DE:** Discipline elective

Criteria of evaluation for theory:

A: Continuous Assessment: [25 Marks]

(i). Surprise Tests (minimum three)-Based on Objective Type Tests (10 marks)

(ii). Term paper (10 marks)

(iii). Assignments (5 marks).

B: Mid-Semester Test – I: Based on Subjective Type Test [25 Marks]

C: Mid-Semester Test – II: Based on Subjective Type Test [25 Marks]

D: End-Term Exam (Final): Online Objective Type Test [25 Marks]

E: Total Marks

Evaluation criteria for practical:

Item	Synopsis	Experiment	Practical Note book and day to day evaluation	Viva voce
Marks	10	10	20	10

SEMESTER IV

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr
1	CMC.571	Organic Chemistry - IV	C	4	-	-	4
2	CMC.572	Green Chemistry	C	3	1	-	4
3	CMC.573	Medicinal Chemistry-III	C	4	-	-	4
4	CMC.574	Organic Chemistry Worksheet-I (DEC-I)	CF (DEC)	2	-	-	2
5	CMC.575	Organic Chemistry Worksheet-II (DEC-II)	CF (DEC)	2	-	-	2
6	CMC.599	Project	SB	-	-	-	6
		Total		15	1	-	22

Any MOOC course of 4 credits or two courses of 2 credits each may be taken

CF: Compulsory Foundation, **C:** Core, **ID:** Interdisciplinary, **DE:** Discipline elective

L: Lectures T: Tutorial P: Practical Cr: Credits

Criteria of evaluation for theory:

A: Continuous Assessment: [25 Marks]

(i). Surprise Tests (minimum three)-Based on Objective Type Tests (10 marks)

(ii). Term paper (10 marks)

(iii). Assignments (5 marks).

B: Mid-Semester Test – I: Based on Subjective Type Test [25 Marks]

C: Mid-Semester Test – II: Based on Subjective Type Test [25 Marks]

D: End-Term Exam (Final): Online Objective Type Test [25 Marks]

E: Total Marks

Evaluation criteria for practical:

Item	Synopsis	Experiment	Practical Note book and day to day evaluation	Viva voce
Marks	10	10	20	10

Semester 1

Course Title: Computer Applications

Paper Code: CST.501

L	T	P	Cr
2	-	-	2

Learning Outcomes:

Upon successful completion of this course, the student will be able to:

1. Use different operating system and their tools easily.
2. Use word processing software, presentation software, spreadsheet software and latex.
3. Understand networking and internet concepts.
4. Use computers in every field like teaching, industry and research.

Unit 1

7 hours

Computer Fundamentals: Introduction to Computer, Input devices, Output Devices, Memory (Primary and Secondary), Concept of Hardware and Software, C.P.U., System bus, Motherboard, Ports and Interfaces, Expansion Cards, Ribbon Cables, Memory Chips, Processors, Software: Types of Software, Operating System, User Interface of popular Operating System, Introduction to programming language, Types of Computer.

Unit 2

8 hours

Computer Network: Introduction to Computer Network, Types of Network: LAN, WAN and MAN, Topologies of Network, Internet concept, WWW.

Word Processing using MS Word: Text creation and Manipulation; Table handling; Spell check, Hyper-linking, Creating Table of Contents and table of figures, Creating and tracking comments, language setting and thesaurus, Header and Footer, Mail Merge, Different views, Creating equations, Page setting, Printing, Shortcut keys.

Unit 3

8 hours

Presentation Tool: Creating Presentations, Presentation views, Working on Slide Transition, Making Notes Pages and Handouts, Drawing and Working with Objects, Using Animations, Running and Controlling a Slide Show, Printing Presentations, Shortcut keys.

Spread Sheet: Entering and editing data in cell, Basic formulas and functions, deleting or inserting cells, deleting or inserting rows and columns, printing of Spread Sheet, Shortcut keys.

Unit 4**7 hours**

Use of Computers in Education and Research: Data analysis tools, e-Library, Search engines related to research such as Protein Data Bank, PubMed, NISCAIR, ACS, RSC, Elsevier, SciFinder, Google Scholar, Google patent, Espacenet, Beilstein databases etc., Research paper editing tools like Latex. Bibliography management and research paper formatting using reference software EndNote and reference manager. Sketching of molecules using ChemBio Draw, ChemSketch etc.

Suggested Readings:

1. Sinha, P. K., & Sinha, P. (2010). *Computer fundamentals* (Vol. 4). BPB publications.
2. Gookin, D. (2013). *Word 2013 for dummies*. John Wiley & Sons.
3. Harvey, G. (2016). *Excel 2016 for dummies*. John Wiley & Sons.
4. Bott, E., Siechert, C., & Stinson, C. (2009). *Windows 7 inside out*. Pearson Education.
5. Goel, A., & Ray, S. K. (2012). *Computers: Basics and Applications*. Pearson Education India.
6. Melton, B., Dodge, M., Swinford, E., & Couch, A. (2013). *Microsoft Office Professional 2013 step by step*. Pearson Education.

Course Title: Organic Chemistry-I**Paper Code: CMC.506**

L	T	P	Cr
4	-	0	4

Learning Outcomes:

Students who successfully complete this course will be able to:

- Understand the stereochemistry, spatial arrangement of atoms/groups and apply it on the course of reactions and mechanism prediction.
- Understand the basics of organic chemistry and enable students to apply knowledge in drug synthesis and their interaction with receptors

Unit 1**18 hours**

Stereochemistry: IUPAC nomenclature of organic molecules, Elements of symmetry, Chirality, Projection formulae [Flywedge, Fischer, Newman and Saw horse], Configurational and conformational isomerism in acyclic and cyclic compounds; Stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, racemic mixture and their resolution, Configurational notations of simple molecules, D/L, R/S, E/Z and cis/trans configurational

notations, Threo and erythro isomers, Methods of resolution, Optical purity, Enantiotopic and diastereotopic atoms, groups and faces, Stereospecific and stereoselective synthesis, Asymmetric synthesis, Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), Chirality due to helical shape, Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus, Conformational analysis of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2-; 1,3-, 1,4-disubstituted cyclohexane derivatives and D-Glucose, Effect of conformation on the course of rate of reactions, Effect of conformation on reactivity, Conformation of sugars, strain due to unavoidable crowding, .

Unit 2

16 hours

Aliphatic nucleophilic substitution reaction: The SN^2 , SN^1 , mixed SN^2 and SN^1 and SET mechanism, The SN^i mechanism. Nucleophilic substitution at an allylic, aliphatic and vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity, competition between SN^2 and SN^1 mechanisms.

Aromatic nucleophilic substitution: The SN^{Ar} , bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, *ortho/para* ratio, ipso attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles, Diazonium coupling, Vilsmeier-Haack reaction.

Unit 3

14 hours

Elimination reactions: E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation.

Unit 4

12 hours

Addition to carbon -hetero multiple bonds: Reactivity of carbonyl group, homologation and dehomologation of carbonyl compounds, nucleophilic addition of hetero-atoms (N,O,S), conjugate addition reactions, acylation of carbonyl carbon, carbonyl cyclizations and cleavages, carboxylic acids and derivatives, decarboxylation reactions, addition of Grignard, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, hydrolysis of esters and amides, ammonolysis of esters.

Suggested Readings:

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry Organic Chemistry* Oxford press, 2nd edition
2. Finar, I.L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
3. Mc Murry J., *Organic Chemistry*, Asian Book Pvt. Ltd, 8th edition, New Delhi
4. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
5. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, New Delhi-110002.
6. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age International (P) Ltd., 5th edition, New Delhi.
7. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
8. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., 3rd edition, New Delhi.
9. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
10. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, New York.
11. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
12. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., 3rd edition, New Delhi.
13. Roberts, J. D., & Caserio, M. C. (1977). *Basic principles of organic chemistry*. WA Benjamin, Inc..
14. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc., 10th edition.
15. Sykes, P. (1986). *A guidebook to mechanism in organic chemistry*. Pearson Education India.
16. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

Course Title: Organic Synthesis –I (Practical)

L	T	P	Cr
-	-	4	2

Paper Code: CMC.507**Learning Outcomes:**

Students who successfully complete this course will be able to:

- Understand stereochemistry of organic compounds
- Handling, storage and disposal of hazardous chemicals and their Material safety data sheets (MSDS)
- Monitoring the progress of chemical reactions by thin layer chromatography
- Purification of a given organic compound through crystallization, fractional distillation or column chromatography
- Basics of Organic Synthesis

Course content:

1. Awareness to various glasswares and plasticwares used in the organic synthesis.
2. Demonstration of Stereochemical aspects of the compounds through molecular models
3. Awareness to handling, storage and disposal of hazardous chemicals and their Material safety data sheets (MSDS).
4. Thin layer chromatography: Monitoring the progress of chemical reactions, identification of unknown organic compounds by comparing the R_f values of known standards, preparative TLC for separation of mixtures
5. Purification of a given organic compound through crystallization, fractional distillation or column chromatography.
6. **Organic Synthesis:** Single or multi- steps synthesis of organic compounds. Aspects such as conversion, yield, selectivity, effluent treatment, atom economy, etc. should be paid attention. TLC should be used to monitor the reaction. (attempt any five)
 - a) Synthesis of an anticancer stilbene via Wittig reaction
 - b) Synthesis of chalcones via Claisen-Schmidt condensation.
 - c) Preparation of vanillyl alcohol from vanillin
 - d) Reduction of 3-nitroacetophone using $\text{NaBH}_4/\text{LiAlH}_4$
 - e) Preparation of bromohydrin from methylstyrene
 - f) Preparation of aniline from nitrobenzene
 - g) Synthesis of ethyl *N*-butylacetoacetate by A.E.E. condensation
 - h) Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.
 - i) Preparation of Iodoxybenzoic acid (IBX) and its application in oxidation.
 - j) Preparation of pyridine chlorochromate (PCC) and its application in oxidation.
 - k) Multistep synthesis of phenytoin.

Evaluation criteria:

Item	Synopsis	Experiment	Practical Note book and day to day evaluation	Viva voce
Marks	10	10	20	10

Suggested Readings:

1. Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan Limited, London.
2. Mann, F. G. (2009). *Practical organic chemistry*. Pearson Education India.
3. Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
4. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranhart and Winston Inc., New York.
5. Vogel, A.I. (latest edition). *Text book of practical organic chemistry*, Pearson
6. Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D. Cand Co., Lexington, MA.
7. Armarego, W. L., & Chai, C. (2012). *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
8. Young, J. A. (Ed.). (1991). *Improving safety in the chemical laboratory: a practical guide*. Wiley.

Course Title: Modern Spectral & Chromatographic Techniques**Paper Code: CMC.508**

L	T	P	Cr
4	-	-	4

Learning Outcomes

- Understanding of the general principle and theory of spectroscopy
- Describe the concept and instrumentation of UV-Vis, IR, NMR, Mass and Chromatographic techniques
- To study the spectra of the compounds and propose structure of the compounds
- Separation and identification of constituents of mixture by chromatographic techniques

Unit 1

18 hours

UV-Visible spectroscopy: Introduction, Theory, Laws, Instrumentation associated with UV-Visible spectroscopy, Choice of solvents and solvent effect and Applications of UV-Visible spectroscopy, Difference/ Derivative spectroscopy.

IR spectroscopy: Theory, Modes of Molecular vibrations, Sample handling, Instrumentation of Dispersive and Fourier – Transform IR Spectrometer, Factors affecting vibrational frequencies and Applications of IR spectroscopy, Data Interpretation.

Spectrofluorimetry: Theory of Fluorescence, Factors affecting fluorescence (Characteristics of drugs that can be analysed by fluorimetry), Quenchers, Instrumentation and Applications of fluorescence spectrophotometer.

Flame emission spectroscopy and Atomic absorption spectroscopy: Principle, Instrumentation, Interferences and Applications.

Unit 2

15 hours

NMR spectroscopy: Quantum numbers and their role in NMR, Principle, Instrumentation, Solvent requirement in NMR, Relaxation process, NMR signals in various compounds, Chemical shift, Factors influencing chemical shift, Spin-Spin coupling, Coupling constant, Nuclear magnetic double resonance, Brief outline of principles of FT-NMR and ¹³C NMR. Applications of NMR spectroscopy.

Mass Spectroscopy: Principle, Theory, Instrumentation of Mass Spectroscopy, Different types of ionization like electron impact, chemical, field, FAB and MALDI, APCI, ESI, APPI Analyzers of Quadrupole and Time of Flight, Mass fragmentation and its rules, Meta stable ions, Isotopic peaks and Applications of Mass spectroscopy.

X ray Crystallography: Production of X rays, Different X ray methods, Bragg's law, Rotating crystal technique, X ray powder technique, Types of crystals and applications of X-ray diffraction.

Unit 3

15 hours

Chromatography: Principle, apparatus, instrumentation, chromatographic parameters, factors affecting resolution, isolation of drug from excipients, data interpretation and applications of the following: Thin Layer chromatography, High Performance Thin Layer Chromatography, Ion exchange chromatography, Column chromatography, Gas chromatography, High Performance Liquid chromatography, Ultra High Performance Liquid chromatography, Affinity chromatography, Gel Chromatography

Electrophoresis: Principle, Instrumentation, Working conditions, factors affecting separation and applications of the following: a) Paper electrophoresis

b) Gel electrophoresis c) Capillary electrophoresis d) Zone electrophoresis e) Moving boundary electrophoresis f) Isoelectric focusing

Unit 4

12 hours

Thermal Techniques: Principle, thermal transitions and Instrumentation (Heat flux and power-compensation and designs), Modulated DSC, Hyper DSC, experimental parameters (sample preparation, experimental conditions, calibration, heating and cooling rates, resolution, source of errors) and their influence, advantage and disadvantages, pharmaceutical applications. Differential Thermal Analysis (DTA): Principle, instrumentation and advantage and disadvantages, pharmaceutical applications, derivative differential thermal analysis (DDTA). TGA: Principle, instrumentation, factors affecting results, advantage and disadvantages, pharmaceutical applications

Potentiometry: Principle, working, Ion selective Electrodes and Application of potentiometry.

Suggested readings

1. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). *Spectrometric identification of organic compounds*. John Wiley & Sons.
2. Skoog, Douglas A. Título: *Principles of instrumental analysis* / Douglas A. Skoog, F.
3. James Holler, Timothy A. Nieman. P. imprenta: Madrid, Esp.: McGRAW HILL. *Instrumental methods of analysis* – Willards, 7th edition, CBS publishers.
4. Beckett, A. H., & Stenlake, J. B. (Eds.). (1988). *Practical Pharmaceutical Chemistry: Part II*. Fourth Edition (Vol. 2). A&C Black..
5. Kemp, W. (1991). *Organic spectroscopy* (pp. 42-51). London: Macmillan.
6. Sethi, P. D. (1985). *Quantitative analysis of drugs in pharmaceutical formulations*. Unique Publishers.
7. Munson, J. W. (Ed.). (1984). *Pharmaceutical analysis: modern methods* (Vol. 11). CRC Press.
8. Kalsi, P. S. (2007). *Spectroscopy of organic compounds*. New Age International.
9. Connors, K. A. (2007). *A textbook of pharmaceutical analysis*. John Wiley & Sons.

Course Title: Spectral Analysis (Practical)
Paper Code: CMC.509

L	T	P	Cr
-	-	4	2

Learning Outcomes

Students who successfully complete this course will be able to:

- Structure elucidation of unknown compounds *via* spectral interpretation of ^1H , ^{13}C NMR, IR, UV and Mass.
- Independent operation of analytical instruments such as FT-IR, UV-vis spectrophotometer, GC-MS, and HPLC

Course content

- Estimation of elements and functional groups in organic natural compounds
- Analysis of organic compounds by UV Vis spectrophotometer
- Experiments based on Column chromatography
- Experiments based on HPLC
- Experiments based on Gas Chromatography
- Characterization of organic compounds using TLC, melting point, ^1H , ^{13}C NMR, IR, UV and Mass.
- Isolation, characterization like melting point, mixed melting point, molecular weight determination, functional group analysis, co-chromatographic technique for identification of isolated compounds and interpretation of UV and IR data

Evaluation criteria:

Item	Synopsis	Experiment	Practical Note book and day to day evaluation	Viva voce
Marks	10	10	20	10

Suggested Readings

1. Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan Limited, London.
2. Mann and Saunders. (2009). *Practical organic chemistry*, Pearson.
3. Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
4. Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
5. Vogel, A.I. (latest edition). *Text book of practical organic chemistry*, Pearson

6. Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D.C and Co., Lexington, MA.
7. Armarego, W. L., & Chai, C. (2012). *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
8. Young, J. A. (Ed.). (Latest Edition). *Improving safety in the chemical laboratory: a practical guide*. Wiley

Course Title: Medicinal Chemistry-I
Paper Code: CMC.510

L	T	P	Cr
3	1	0	4

Learning Outcomes

Students who successfully complete this course will be able to:

- Understand basics concepts of drugs, their effects and screening.
- Know how drugs interact with various types of enzymes and receptors
- Know the process of drug discovery and its progress.

Unit 1

12 hours

History of drug discovery: Introduction, Drug discoveries, Recent trends in drug discovery. Enzymes as drug targets, Membrane transporters as drug targets, Voltage-gated ion channels as drug targets

Unit 2

17 hours

Medicinal chemistry: Definitions and objectives, Drug activity phases, Drug classification system.

Measurement and expression of drug effects: Introduction, *In-vitro* experiments, *Ex-vivo* experiments, *In-vivo* experiments.

Unit 3

15 hours

Molecular drug targets: Introduction, Non-selective cation-channels as drug targets, Direct ligand gated ion channels, Receptors with intrinsic enzyme activity, Receptors coupled to various cytosolic proteins, G-Protein coupled receptors, Nuclear receptors.

Unit 4

16 hours

Drug targets, target identification, validation and screening: Introduction, Improving the resolution of disease etiology, Biopharmaceutical therapies, Drug target identification, Hit to lead, Clinical biomarkers.

Suggested Readings:

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., Philadelphia.
2. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, Philadelphia.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royal Society of Chemistry, Second Edition.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, Third Edition.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Publisher: I.K. International Pvt. Ltd.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, Fourth Edition.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
9. Wolff, M E, Ed., (Latest Edition). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley and Sons, New York.

Elective courses

Course Title: Chemistry of Natural Products

L	T	P	Cr
4	-	-	4

Paper Code: CMC.511

Learning Outcomes

- Students will become familiar with various types of natural products
- Students will understand the role of natural products in living organisms, their biosynthesis and will have a greater understanding of organic synthesis
- To understand the role of natural products in drug discovery and development

Unit 1

15 hours

Terpenoids and carotenoids: Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule. Structure

determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Geraniol, Menthol and β -Carotene

Unit 2

15 hours

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, Nicotine and Morphine.

Unit 3

15 Hours

Steroids: Occurrence, nomenclature, basic skeleton and stereochemistry, Structure determination and synthesis of cholesterol, partial synthesis of Testosterone and Progesterone, Chemical tests for steroids

Unit 4

15 Hours

Flavonoids: Introduction, isolation and purification of flavonoids, General methods of structural determination of flavonoids; Structural elucidation of quercetin

Structural Characterization of natural compounds: Structural characterization of natural compounds using IR, ^1H NMR, ^{13}C NMR and MS Spectroscopy of specific drugs e.g., Penicillin, Morphine, Camphor, Vit-D, Quercetin and Digitalis glycosides.

Suggested Readings

1. Bhat, S.V., Nagasampagi, B.A., Meenakshi, S. (2009). *Natural Product Chemistry & Applications*, Narosa Publishing House, New Delhi.
2. Bhat, S.V., Nagasampagi, B.A., Sivakumar, M. (2005), *Chemistry of Natural Products*. Narosa Publishing House, New Delhi.
3. Brahamchari, G. (2009). *Natural Product: Chemistry, Biochemistry and Pharmacology*. . Narosa Publishing House, New Delhi.
4. Cseke, L.J. (2009). *Natural Products from plants*. CRC Press, Taylor and Francis, 2nd edition, US.
5. Dewick, P.M. (2009). *Medicinal Natural Products: A Biosynthetic Approach*. Willey & Sons, 3rd edition, UK.
6. Finar, I.L. (2006). *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*. Dorling Kindersley Pvt. Ltd., 6th edition, India.
7. Peterson, F., Amstutz, R. (2008). *Natural Compounds as drugs*. Birkhauser Verlay.
8. Thomson, R.H. (2008). *The Chemistry of Natural Products*, Springer, 1st edition.

Course Title: Quantum Chemistry
Paper Code: CMC.512

L	T	P	Cr
4	-	-	4

Learning Outcomes

Students who successfully complete this course will be able to learn about:

- Quantum chemical description of chemical bonding, reactivity and their applications in molecular spectroscopy and inorganic chemistry
- Schrodinger equation for a particle in a box and quantum chemical description.
- Electronic and Hamiltonian operators for molecules.
- Quantum chemical description of angular momentum and term symbols for a one and many-electron systems.
- Born-Oppenheimer approximation, the Pauli principle, Hund's rules, Hückel theory and the variation principle

Unit 1

15 hours

Fundamental Background: Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor, Particle in a Ring, Hydrogen Atom.

Unit 2

15 hours

Approximate Methods: Perturbation theory for non-degenerate and degenerate states and its applications. The variation theorem and its application.

Unit 3

15 hours

Angular Momentum: Ordinary angular momentum, Eigen functions and Eigen values for angular momentum, Addition of angular momenta, Spin, Antisymmetry and Pauli exclusion principle.

Electronic Structure of Atoms: Electronic configuration, Russell-Saunders terms and Coupling Schemes, Magnetic Effects: Spin-orbit Coupling and Zeeman Splitting, the self-consistent field method, Hartree-Fock SCF method for molecules.

Unit 4

15 hours

Born-Oppenheimer Approximation: LCAO-MO and VB treatments of the H_2^+ and H_2 , Hybridization and valence MOs of H_2O and NH_3 . Huckel Theory of acyclic and cyclic conjugated systems, Bond Order and Charge Density Calculations.

Suggested Readings

1. Levine, I.N. *Quantum Chemistry*, 5th edition, 2000, Pearson Educ., Inc. New Delhi.
2. Chandra, A.K. *Introductory Quantum Chemistry*, 4th Edition, 1994, Tata Mcgraw Hill.
3. Prasad, R.K., *Quantum Chemistry*, 4th Edition, 2009, New Age Science.
4. Mcf Quarrie, D. A. (1997). *Physical Chemistry: A molecular approach* (No. 539 M34).
5. Murrell, J.N. Kettle S.F.A. and Tedder, J. M. *Valence Theory*, 2nd edition, 1965, John Wiley.
6. Lowe, J. P. and Peterson, K. *Quantum Chemistry*, 3rd Edition, 2006, Academic Press.

Semester -2

Course Title: Organic Chemistry-II

Paper Code: CMC.521

L	T	P	Cr
4	-	0	4

Learning Outcomes

Students who successfully complete this course will be able to:

- Understand the disconnection approaches apply it on synthetic strategies and mechanism prediction.
- Understand the basics of photochemical reactions that will enable understand students to build knowledge in drug synthesis

Unit 1

12 hours

Reactive intermediates: Generation, structure and reactions of carbocation, carbanion, free radicals, carbenes, nitrenes, benzynes, classical and non-classical carbocations, phenonium ions and norbornyl system, neighbouring group participation.

Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.

Unit 2

17 hours

Synthetic methodologies: Synthon, Synthetic equivalent, Functional group interconversion (FGI), Functional group addition, Functional group elimination, Criteria for selection of target, Linear and convergent synthesis, Retrosynthetic analysis and synthesis involving chemoselectivity, Regioselectivity, Reversal of Polarity (Umpolung), Synthesis of cyclic molecules, Strategic bond: Criteria for disconnection of strategic bonds, Importance of the order of events in organic synthesis. One group and two group C-X disconnections in 1,2-, 1,3-, 1,4 & 1,5- difunctional compounds, One group C-C disconnections, alcohol and carbonyl compounds, regioselectivity, alkene synthesis, use of acetylenes and

aliphatic nitro compounds in organic synthesis, Two group C-C disconnections, Diels-Alder reaction, 1,3-difunctionalised compounds, Control in carbonyl condensation, 1,5-difunctionalised compounds.

Unit 3

13 hours

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, Mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzilic acid, Favorskii, Arndt-Eister synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction, Carroll, Claisen, Cope, Gabriel-Colman, Smiles and Sommelet-Hauser rearrangements.

Selective Name Reactions: Aldol, Perkin, Stobbe, Dieckmann Condensation, Reimer-Tiemann, Reformatsky Grignard reactions, Diels-Alder reaction, Robinson Annelation, Michael addition, Mannich reaction, Stork-enamine, Sharpless Assymetric Epoxidation, Ene, Barton, Hofmann-Loffler Fretag, Shapiro reaction, Chichibabin Reaction.

Unit 4

18 hours

Pericyclic chemistry:

Introduction, Main features of pericyclic reactions, Classification of pericyclic reactions. Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1, 3-butadiene, 1,3,5- hexatriene. Allyl cation, allyl radical, pentadienyl cation and pentadienyl radical. Thermal and photochemical pericyclic reactions.

Electrocyclic reactions: Conrotation and disrotation, Electrocyclic closure and opening in $4n$ and $4n+2$ systems. Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by (i) symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and orbital symmetry correlation diagrams and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Examples of electrocyclic reactions.

Cycloaddition reactions: Suprafacial and antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Cycloreversions. Stereochemical aspects in supra-supra, supra-antara, antara-supra and antara-antara $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Diels-Alder reaction. Woodward-Hoffmann Selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by (i) Conservation of orbital symmetry and orbital symmetry correlation diagrams (ii) Fukui Frontier Molecular Orbital (FMO) theory and (iii) Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Examples of cyclo addition reactions.

Sigmatropic reactions: $[1,j]$ and $[i,j]$ shifts; Suprafacial and antarafacial shifts; Selection rules for $[l,j]$ shifts; Cope and Claisen rearrangements; Explanation for the mechanism of sigmatropic reactions by (i) symmetry properties of HOMO (ii)

Introduction to Cheletropic reactions and the explanation of mechanism by FMO theory.

Suggested Readings

1. Morrin Acheson, R. An introduction to the chemistry of heterocyclic compounds. (2008)Wiley India Pvt. Ltd., 3rd edition.
2. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry Organic Chemistry* Oxford press, 2nd edition
3. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, India.
4. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
5. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age International (P) Ltd., 5th edition, New Delhi.
6. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (P) Ltd., 5th edition, New Delhi.
7. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B*, Springer, 5th edition.
8. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
9. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, US.
10. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
11. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, 5th edition, New York.
12. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3rd edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.

18. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, US.
19. Norman, R.O.C.; Coxon, J.M. *Principles of Organic Synthesis*, Blackie Academic & Professional.
20. Warren, S., (2010). *Organic synthesis: The Synthons Approach*. John Wiley & Sons, New York,
21. Warren, S., (2010). *Designing organic synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
22. Corey E.J., Cheng Xue-Min, *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons, (1989).

Course Title: Organic Synthesis-II (Practical)

L	T	P	Cr
-	-	4	2

Paper Code: CMC.522

Learning Outcomes

Students who successfully complete this course will be able to:

- Separation of mixture of *ortho* and *para* mixture and cis/trans mixture by column chromatography
- Multi-Step Synthesis of Organic Compounds
- Identification of compounds *via* combined spectral interpretation of ¹H, ¹³C NMR, IR, UV and Mass along with 2-D NMR spectra.

Course content

1. Separation and purification of organic compounds by column chromatography: Separation of mixture of *ortho* and *para* mixture and cis/trans mixture. The column chromatography should be monitored by TLC.
2. **Multi-Step Synthesis of Organic Compounds:** The exercise should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques. (Any five)
 - a) Synthesis of isoxazole derivatives via 1,3-dipolar cycloaddition.
 - b) Synthesis of pyrazole derivatives from chalcones.
 - c) Synthesis of an antihypertensive drug-propranolol via epoxide ring opening reaction.
 - d) Synthesis of Diltiazem (a calcium channel blocker) via Darzen condensation, a key step in its synthesis.
 - e) Protection and deprotection of alcohols and amines.
 - f) Preparation of Triphenyl Carbinol from Bromobenzene (Grignard's reaction)
 - g) Preparation of allylic alcohols via Baylis-Hillman reaction using DABCO as a catalyst under neat condition and their characterization through various spectroscopic techniques.

- h) Preparation of homoallyl alcohols via Barbier type reaction under aqueous condition using Indium as a catalyst.
- i) Suzuki reaction of 3,4-dimethoxy phenyl boronic acid with aryl halides using Pd(PPh₃)₄ as a catalyst.
3. Exercises on identification of compounds *via* combined spectral interpretation of ¹H, ¹³C NMR, IR, UV and Mass along with 2-D NMR spectra.

Evaluation criteria

Item	Synopsis	Experiment	Practical Note book and day to day evaluation	Viva voce
Marks	10	10	20	10

Suggested Readings

- Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan Limited, London.
- Mann and Saunders. (2009). *Practical organic chemistry*, Pearson.
- Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
- Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
- Vogel, A.I. (Latest edition). *Text book of practical organic chemistry*, Pearson
- Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D.Cand Co.,Lexington, MA.

Course Title: Basics of Drug Design and Drug Actions

Paper Code: CMC.523

L	T	P	Cr
4	-	0	4

Learning outcome: Students who successfully complete this course will be able to

- Apply the knowledge of drug-receptor interactions for understanding drug mechanism
- Utilize the knowledge of ligand interactions with the active site of receptor in novel drug design and discovery
- Apply the knowledge on QSAR for novel drug designing

Unit 1

12 hours

Interactions of enzyme/receptor with drug molecules; Chirality and drug action; Covalent, ion-dipole, hydrogen bonding, C-H hydrogen bonding, dihydrogen bonding, van der waals interactions and the associated energies, Receptor & biological response, Drug-receptor interactions, receptor theories and drug action, Occupancy theory, rate theory, induced fit theory, macromolecular perturbation theory, activation-aggregation theory. Topological and stereochemical consideration.

Theoretical Aspects of Drug Action: Drug distribution, Active transport, Passive transport, The Ferguson Principle Physicochemical Parameters and Pharmacological Activity-Solubility, Partition Coefficient, Surface Activity, pKa, Ionisation, Stereochemical Factors, Bio-isosterism.

Unit 2

12 hours

Enzyme kinetics in drug action: Mechanisms of enzyme catalysis, Electrostatic catalysis and desolvation, Covalent catalysis, acid-base catalysis, strain / distortion in enzyme catalysis, Coenzyme catalysis, Theories of enzyme inhibition and inactivation, Enzyme activation of drugs-prodrugs.

Drug metabolism: Metabolic Processes- Phase-I (Oxidation, Reduction & Hydrolysis) and Phase-II (Glucuronide Conjugation, Acetylation, Methylation, Sulphate Conjugation, Conjugation with amino acids and Mercapturic acid formation), Routes of Elimination, Factors Affecting Metabolism-Genetic Factors, Physiological Factors, Pharmaceutical Factors, Drug Interactions.

Unit 3

20 hours

SAR studies, Lead modification and Drug Design: Lead modification strategies; Bioisosterism, variation of alkyl substituents, chain homologation and branching, Variation of aromatic substituents, Extension of structure,

Ring expansion or contraction, Ring variation, Variation in position of hetero atoms, Ring fusion, Simplification of the lead, Rigidification of lead; Discovery of oxamiquine, salbutamol, cimitidine and captopril. Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, barbiturates, and taxol analogs. Principles of prodrug design, Serendipitous discovery of leads e.g. Penicillin and librium, sildenafil.

In silico methods: Introduction to Quantitative Structure Activity Relationship (QSAR) studies. 2-D QSAR, QSAR parameters. 3-D QSAR, CoMFA and CoMSIA. Molecular docking, Pharmacophore mapping and virtual screening.

Unit 4

16 hours

Combinatorial synthesis and chiral drugs: Introduction, Combinatorial approach. Combinatorial library, Solid phase synthesis, resins, linkers. Parallel synthesis; Haughton's tea bag procedure, Automated parallel synthesis, Mix and Split combinatorial synthesis, Structure determination of active compounds, Synthesis of heterocyclic combinatorial libraries, Analytical characterization of synthetic organic libraries.

Suggested Readings

1. Ellis, G.P., West, G. B. (1983). *Progress in Medicinal Chemistry Series*. Elsevier Science.
2. Foye, W.O.; Lemke, T. L.; Williams, D. A. (Latest Edition). *Principles of Medicinal Chemistry*, Indian Ed. Waverly, Pvt. Ltd. New Delhi.
3. Ganellin, C.R.; Roberts S. M., (1993). *Medicinal Chemistry: The Role of Organic Chemistry in Drug Research*. Publisher: Academics Press Inc.
4. Kadam, Mahadik, Bothara (2010). *Principle of Medicinal Chemistry (Volume I & II)*, Nirali publication
5. Kulkarni, V. M., Bothra, K.G., (2008). *Drug Design*, Nirali Publication.
6. Lawton, G., Witty, D.R. (2011). *Progress in Medicinal Chemistry Series. Volume 50*.
7. Lednicer D., Laster A. M. (1998). *The Organic Chemistry of Drug Synthesis(3 Volumes)* John Wiley & Sons.
8. Lednicer, D. (2008). *Strategies for Organic Drug Synthesis and Design. (7 volume)* Publisher: John Wiley & Sons.
9. Lemke, T.L., Williams, D.A. (2012). *Foye's Principles of Medicinal Chemistry*. 7th edition.
10. Silverman R.B., (2014). *Organic Chemistry of Drug Design and Drug Action*, Publisher: Elsevier.
11. Wilson, C.O.; Block, J.H.; Gisvold, O.; Beale, J. M. Wilson and Gisvold's (2003) *Textbook of Organic Medicinal and Pharmaceutical Chemistry*. Lippincott Willaiams & Wikins.

Course Title: Computer Aided Drug Design - Practical

Paper Code: CMC.524

L	T	P	Cr
-	-	4	2

Learning outcome: Students who successfully complete this course will be able to

- Determine log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares
- Calculation of ADMET properties of drug molecules and its analysis using softwares
- Pharmacophore modeling
- Perform 2D-QSAR based experiments
- Perform 3D-QSAR based experiments
- Perform Docking study based experiment
- Perform virtual screening based experiment
- Perform Homology Modelling based experiments.

Course content:

Following practicals utilizing the available softwares such as ChemBio Draw, Autodock, Schrodinger, etc. need to be conducted.

- 1) Determination of log P, MR, hydrogen bond donors and acceptors of selected drugs using softwares
- 2) Calculation of ADMET properties of drug molecules and its analysis using softwares
- 3) Pharmacophore modeling
- 4) 2D-QSAR based experiments
- 5) 3D-QSAR based experiments
- 6) Docking study based experiment
- 7) Virtual screening based experiment
- 8) Homology Modelling based experiments.
- 9) Practical based on 2D and 3D-QSAR of drug molecules.
- 10) Docking and virtual screening based experiments.

Evaluation criteria:

Item	Synopsis	Experiment	Practical Note book and day to day evaluation	Viva voce
Marks	10	10	20	10

Suggested Readings

1. León, D.; Markell S. *In silico Technologies in Drug Target Identification and Validation*. 2006 by Taylor and Francis Group, LLC.
2. Kubiny, H. *QSAR: Hansch Analysis and Related Approaches. Methods and Principles in Medicinal Chemistry*. Publisher Wiley-VCH
3. Gubernator, K.; Böhm, H. *Structure-Based Ligand Design. Methods and Principles in Medicinal Chemistry*. Publisher Wiley-VCH
4. Parrill, A. H.; Reddy, M R. *Rational Drug Design. Novel Methodology and Practical Applications*.
5. Turner J. R. *New drug development design, methodology and, analysis*. John Wiley & Sons, Inc., New Jersey.

Course Title: Advanced Spectral Analysis
Paper Code: CMC.525

L	T	P	Cr
4	-	0	4

Learning outcome: Students who successfully complete this course will be able to

- Understand hyphenated analytical instrumental techniques for identification, characterization and quantification of drugs. Instruments dealt are LC-MS, GC-MS, ATR-IR, DSC etc.
- Interpretation of the NMR, Mass and IR spectra of various organic compounds
- Theoretical and practical skills of the hyphenated instruments
Identification of organic compounds

Unit 1

15 Hours

UV and IR spectroscopy: Woodward – Fieser rule for 1,3-butadienes, cyclic dienes and α , β -carbonyl compounds and interpretation of enones.
ATR-IR, IR Interpretation of organic compounds.

Raman Spectroscopy: Introduction, Principle, Instrumentation and Applications.

Unit 2

15 Hours

NMR spectroscopy: 1-D and 2-D NMR, NOESY and COSY, HECTOR, INADEQUATE techniques, Interpretation of organic compounds.

Thermal methods of analysis: Introduction, principle, instrumentation and application of DSC, DTA and TGA.

Unit 3

15 Hours

Mass Spectroscopy: Mass fragmentation and its rules, Fragmentation of important functional groups like alcohols, amines, carbonyl groups and alkanes, Meta stable ions, McLafferty rearrangement, Ring rule, Isotopic peaks, Interpretation of organic compounds.

Radio immuno assay: Biological standardization, bioassay, ELISA, Radioimmuno assay of digitalis and insulin.

Unit 4

15 Hours

Chromatography: Principle, Instrumentation and Applications of the following :a) GC-MS b) GC-AAS c) LC-MS d) LC-FTIR e) LC-NMR f) CE-MS g) High Performance Thin Layer chromatography h) Super critical fluid chromatography i) Ion Chromatography j) I-EC (Ion-Exclusion Chromatography) k) Flash chromatography

Suggested Readings:

1. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). *Spectrometric identification of organic compounds*. John wiley & sons.
2. Skoog, D. A., Holler, F. J., & Crouch, S. R. (2017). *Principles of instrumental analysis*. Cengage learning.
3. Willard, H. H., Merritt Jr, L. L., Dean, J. A., & Settle Jr, F. A. (1988). *Instrumental methods of analysis*.
4. Kemp, W. (1991). *Organic spectroscopy* (pp. 42-51). London: Macmillan.
5. Sethi, P. D. (1996). *HPTLC: high performance thin-layer chromatography; quantitative analysis of pharmaceutical formulations*. CBS publishers & distributors.
6. Sethi, P. D. (1985). *Quantitative analysis of drugs in pharmaceutical formulations*. CBS Publishers, New Delhi, 1997.
7. Munson, J. W. (Ed.). (1984). *Pharmaceutical analysis: modern methods* (Vol. 11). CRC Press.

Course Title: Seminar

L	T	P	Cr
-	-	-	1

Paper Code: CMC.542

Learning outcome: Students who successfully complete this course will be able to

- Perform literature review on a given topic
- Prepare a report on a given topic
- Prepare a power point presentation on a given topic

Evaluation criteria:

- Literature survey/background information
- Organization of content
- Physical presentation
- Questions and answers
- Report evaluation

Value added Elective Course:**Credit Hours:1.**

These courses may be chosen from a pool of courses designed to provide value-based and/or skill-based knowledge and should contain both theory and lab/hands-on/training/field work. The list of Value added courses is given below:

S. No.	Name of Course
1.	Ethics for Science
2.	Professional Ethics
3.	Academic Writing
4.	Peace and Value Education
5.	Stress Management
6.	Personality Development through Life Skills
7.	Physical & Mental Well Being
8.	Pedagogical Studies
9.	Data Analysis using spread sheet
10.	Soft Skill Training
11.	Leadership
12.	Personal Management
13.	Human Resource Management
14.	Physical resource management
15.	Reasoning Ability
16.	MS office Specialist
17.	Practical Taxation
18.	Ethical Issues & Legal Awareness
19.	Disaster Management
20.	Nutrition and Specialty Foods
21.	Shorthand & Typing
22.	SPSS application

* The student has to choose 1 course in the present semester.

** The list is subject to addition/deletion/modifications at University level.

Semester –3**Course Title: Research Methodology**

L	T	P	Cr
2	-	0	2

Paper Code: CMC.551**Learning Outcomes:**

Students who successfully complete this course will be able to:

- select and define an appropriate research problem and parameter
- Understand, design and set the objectives based on the literature search.
- Grasp the knowledge to prepare poster and dissertation work

Unit 1**7 hours**

General Research Methodology: Research, objective, requirements, practical difficulties, review of literature, study design, types of studies.

Unit 2**8 hours**

General Research Methodology: Strategies to eliminate errors/bias, controls, randomization, crossover design, placebo, blinding techniques.

Unit 3**7 hours**

Entrepreneurship and business development: Technical writing: Scientific writing, Writing research paper, Poster preparation and Presentation and Dissertation.

Unit-4**8 hours**

Library: Classification systems, e-Library, Reference management, Web-based literature search engines

Suggested Readings:

1. Gupta, S. (2005). *Research methodology and statistical techniques*, Deep & Deep Publications (p) Ltd. New Delhi.
2. Kothari, C. R. (2008.) *Research methodology(s)*, New Age International (p) Limited. New Delhi
3. Best J. W., Khan J. V. (Latest Edition) *Research in Education*, Prentice Hall of India Pvt. Ltd.
4. *Safe science: promoting a culture of safety in academic chemical research*; National Academic Press, www.nap.edu.

Course Title: Organic Chemistry-III

L	T	P	Cr
4	-	0	4

Paper Code: CMC.552

Learning outcome: Students who successfully complete this course will be able to:

- Propose and determine the mechanism and feasibility of a chemical reaction
- Apply principle of photochemistry in various chemical transformations
- Explore various metal and non-metal reagents towards oxidation and reduction reactions
- Name different fused and bridged heterocyclic compounds and perform their synthesis through different methods

Unit 1**13 hours**

Reaction mechanism, structure and reactivity: Types of mechanisms, types of reactions, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, Potential energy diagrams, Transition states and intermediates, Kinetics and non-kinetics method, Isotopes effects, Effect of structure on reactivity; Resonance, inductive, electrostatic and steric effect, quantitative treatment, the Hammett equation and linear free energy relationship, Substituent and reaction constants, Taft equation.

Unit 2**13 hours**

Photochemistry: Franck-Condon principle, Jablonski diagram, Singlet and triplet states, Photosensitization, Quantum efficiency, Photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Di π - methane rearrangement.

Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction Singlet molecular oxygen reactions

Unit 3**15 hours**

Metal and non-metal mediated oxidation and reductions: Mechanism, Selectivity, Stereochemistry and applications of oxidation reactions, Oppenauer, Baeyer-Villiger, Oxidation reactions using DDQ, NBS, leadtetraacetate, selenium dioxide, DCC, PCC, CAN, Cr and Mn reagents, periodic acid, Osmium tetroxide, Swern oxidations, Hydroboration, Dehydrogenation, Ozonolysis, Epoxidations using peracids.

Mechanism, selectivity, stereochemistry and applications of catalytic hydrogenations using Pd, Pt and Ni catalysts, Clemmensen reduction, Wolff-

Kishner reduction, Meerwein-Ponndorf-Verley reduction, Dissolving metal reductions, metal hydride reductions using NaBH_4 , LiAlH_4 , DIBAL. Wilkinson's Rh catalysis, Boron in reduction

Unit 4

19 hours

Heterocyclic chemistry: Replacement and systematic nomenclature (Hantzsch-Widman system) for monocyclic, fused and bridged heterocycles, Aromatic heterocycle, Non-aromatic heterocycle: Bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles and their synthesis

- a. Three-membered and four-membered heterocycles: synthesis and reactions of aziridines, oxiranes, thiranes, azetidines, oxetanes and thietanes.
- b. Five membered heterocycles containing two heteroatoms (S,N,O): Diazoles, imidazole, pyrazole, oxazoles and thiazoles.
- c. Benzo-fused five-membered and six membered heterocycles: Synthesis and reactions of indoles, benzofurans and benzimidazoles, benzothiazoles.
- d. Six-membered heterocycles with heteroatom: Synthesis and reactions of pyrylium salts and pyrones, coumarins, chromones, pyridine, pyrimidine etc.

Suggested Readings

1. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3rd edition.
2. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, India.
3. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
4. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age International (P) Ltd., 5th edition, New Delhi.
5. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (P) Ltd., 5th edition, New Delhi.
6. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B*, Springer, 5th edition.
7. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
8. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, US.
9. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.

10. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, 5th edition, New York.
11. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7th edition, India.
12. Kalsi P. S., (2014). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3rd edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7th edition, India.
19. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.
20. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
21. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
22. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.

Course Title: Medicinal Chemistry-II

Paper Code: CMC.553

L	T	P	Cr
4		0	4

Learning outcome: Students who successfully complete this course will be able to

- To know the basic concepts of drugs, their effects and screening
- To know how drugs interact with various types of enzymes and receptors
- To know the mechanism of action and SAR studies of drug molecules

Unit 1

15 Hours

Physicochemical and stereochemical aspects: In relation to biological activity, Drug receptor interaction, Adrenergic hormones and Drugs including

biosynthesis, storage, release and metabolism of catecholamines (Andrenaline, Isoprenaline, Salbutamol, Amphetamine, Naphazoline), Cholinergics and Anticholinesterases including biosynthesis, storage and metabolism of acetylcholine (Methacholine Chloride, Neostigmine Bromide), Antispasmodic and Antiulcer Drugs (Cyclopentolate, Propantheline Bromide, Benzhexol), Antiparkinsonism Drugs (Apomorphine).

Unit 2

15 Hours

Neuromuscular blocking agents: Gallamine Triethiodide, Succinylcholine chloride, Hypoglycaemic drugs (Tolbutamide), Thyroid hormones and Antithyroid drugs (L- Thyroxine, Propylthiouracil) Pancuronium, vecuronium, rocuronium, rapacuronium, dacturionium, malouetine, duador, dipyrandium, pipecuronium, chandonium. Anticoagulants and haemostatic agents: Warfarin, Phenindione, Oxytocics (includes discussion on Ergot alkaloids) (Ergometrine). Antihistamines including discussion on Sodium cromoglycate (Mepyramine, Diphenhydramine, Chlorpheniramine, Promethazine). Non-steroidal anti-inflammatory drugs and anti-gout drugs: Indomethacin, Phenylbutazone, Allopurinol, Probenecid.

Unit 3

15 Hours

General Anaesthetic Agents: Introduction, medicinal aspects of anaesthetics, mode of action, gases and volatile liquid anaesthetics, intravenous anaesthetics or fixed anaesthetics, toxicity of general anaesthetics (Divinyl ether, Ethyl chloride, Cyclopropane, Thiopentone Sodium).

Local Anaesthetic Agents: Introduction, Structure-activity relationships, benzoic acid derivatives, aminobenzoic acid derivatives, lidocaine derivatives, miscellaneous, toxicity, mode of action (Benzocaine, Procaine Hydrochloride, Lidocaine Hydrochloride).

Unit 4

15 Hours

Sedatives-Hypnotics: Introduction, classification of sedative-hypnotics, structure-activity relationships, barbiturates, amides and imides, alcohols and their carbamate derivatives, aldehydes and their derivatives, mode of action, pharmacological properties and side effects (Barbitone, Phenobarbitone, Cyclobarbitone, Pentobarbitone Sodium, Thiopentone Sodium), non-barbiturates (Official drugs).

Anticonvulsants: Introduction, epilepsy and its types, SAR, barbiturates (official products), hydantoins, Oxazolidinediones, Succinamides; miscellaneous drugs, (Phenytoin Sodium, Troxidone), Antipsychotic agents: introduction, SAR and drugs like chlorpromazine, prochlorperazine *etc.*

Suggested Readings

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., Philadelphia.
2. Foye, W. C. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea & Febiger, Philadelphia.
3. King, F. D. (2006). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2nd edition, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3rd edition, UK.
5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4th edition, US.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, 4th edition.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier).
9. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery* John Wiley & Sons, 7th edition, New York.

Course Title: Organic Chemistry-III (Practical)

Paper Code: CMC.554

L	T	P	Cr
-	-	4	2

Learning outcomes: Students who successfully complete this course will be able to do:

- Synthesis of 5, 6, and 7 membered heterocyclics compounds and their characterization
- Metal catalyzed reactions
- Interpretation of UV, IR, ¹H data and ¹³C NMR, IR, UV and Mass spectral data

Course contents:

1. Synthesis of 5, 6, and 7 membered heterocyclics using conventional heating or microwave heating
2. Experiments involving photochemical reactions
3. Experiments involving metal catalyzed reaction
4. Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using UV data

- Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using IR data
- Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using ^1H data
- Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using ^1H data and ^{13}C NMR
- Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using Mass
- Exercises of structure identifications of above synthesized compounds *via* spectral interpretation using combined data of UV, IR, ^1H data and ^{13}C NMR, IR, UV and Mass.

Evaluation criteria:

Item	Synopsis	Experiment	Practical Note book and day to day evaluation	Viva voce
Marks	10	10	20	10

Suggested Readings:

- Adams, R.; Johnson, J.R.; Wilcox, C.F. (1970). *Laboratory Experiments in Organic Chemistry*, The Macmillan Limited, London.
- Mann and Saunders. (2009). *Practical organic chemistry*, Pearson.
- Pasto, D.P., Johnson, C., Miller, M. (2010). *Experiments and Techniques in Organic Chemistry*, Prentice Hall.
- Roberts, R.M.; Gilbert, J.C.; Rodewald, L.B.; Wingrove, A.S. (1969). *An introduction to Modern Experimental Organic Chemistry*, Ranehart and Winston Inc., New York.
- Vogel, A.I. (latest edition). *Text book of practical organic chemistry*, Pearson
- Williamson, K.L., Heath, D.C. (1999). *Macroscale and Microscale Organic Experiments*, Heath, D.C and Co., Lexington, MA.
- Armarego, W. L., & Chai, C. (2012). *Purification of Laboratory Chemicals*. Butterworth-Heinemann.
- Young, J. A. (Ed.). (Latest Edition). *Improving safety in the chemical laboratory: a practical guide*. Wiley

Value added Elective Course**Credit hours:1.**

These courses may be chosen from a pool of courses designed to provide value-based and/or skill-based knowledge and should contain both theory and lab/hands-on/training/field work. The list of Value added courses is given below:

S. No.	Name of Course
1.	Ethics for Science
2.	Professional Ethics
3.	Academic Writing
4.	Peace and Value Education
5.	Stress Management
6.	Personality Development through Life Skills
7.	Physical & Mental Well Being
8.	Pedagogical Studies
9.	Data Analysis using spread sheet
10.	Soft Skill Training
11.	Leadership
12.	Personal Management
13.	Human Resource Management
14.	Physical resource management
15.	Reasoning Ability
16.	MS office Specialist
17.	Practical Taxation
18.	Ethical Issues & Legal Awareness
19.	Disaster Management
20.	Nutrition and Specialty Foods
21.	Shorthand & Typing
22.	SPSS application

* The student has to choose 1 course in the present semester.

** The list is subject to addition/deletion/modifications at University level.

Course Title: Seminar

Paper Code: CMC.543

L	T	P	Cr
-	-	-	1

Learning outcome: Students who successfully complete this course will be able to

- Perform literature review on a given topic
- Prepare a report on a given topic
- Prepare a power point presentation on a given topic

Evaluation criteria:

- Literature survey/background information
- Organization of content
- Physical presentation
- Questions and answers
- Report evaluation

Course Title: Project

Paper Code: CMC.599

L	T	P	Cr
-	-	-	6

Learning outcome: Students who successfully complete this course will be able to

- Design a research problem and prepare synopsis
- Plan and execute experiments in the laboratory
- Interpret and analyze the results

Evaluation criteria:

- Literature survey/background information
- Organization of content
- Physical presentation
- Questions and answers
- Report evaluation

Elective courses

Course Title: Current Trends in Organic Synthesis

Paper Code: CMC.555

L	T	P	Cr
4	-	0	4

Learning Outcomes:

Students who successfully complete this course will be able to:

- Understand the role of free radicals in chemical transformation
- Understand the importance of organometallic compounds and their application
- Apply the knowledge of various reagents for the synthesis of target molecules and will also acquire knowledge of some important C-C, and C-N bond formation reactions

Unit 1

15 hours

Free radical reactions

Types of free radical reactions, free radical substitution mechanism at an aromatic substrate, neighbouring group assistance, Reactivity for aliphatic and aromatic substrates at a bridgehead,

Reactivity in the attacking radicals, The effect of solvents on reactivity, Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation. Coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction, Free Radical Rearrangement, Hunsdiecker reaction

Unit 2

15 hours

Organometallic compounds

Organoboranes: Preparation of Organoboranes viz hydroboration with BH₃-THF, dicyclohexyl borane, disiamyl borane, teryl borane, 9-BBN and disopinacamplyl borane, functional group transformations of Organo boranes- Oxidation, protonolysis and rearrangements. Formation of carbon-carbon-bonds viz organo boranes carbonylation.

Grignard reagents, Organo lithium, Organo zinc, Organo cadmium and Organo Copper Compounds, Organo silicon compounds for organic synthesis, Organopalladium and organostannous (Applications in coupling reactions).

Unit 3

15 hours

Reagents in organic synthesis: Gilman's reagent, Lithium diisopropylamide (LDA), Dicyclohexyl Carbodiimide (DCC), 1,3-Dithiane (Umpolung reagent), Trimethylsilyliodide, Baker's yeast, DDQ, Lead tetraacetate, Prevost Hydroxylation, Wilkinson's catalyst, Phase transfer catalysts: Quaternary ammonium and Phosphonium salts, Crown ethers, Merfield resin, Fenton's

reagents, Ziegler-Natta catalyst, Lawson reagents, K-selecteride and L-selecteride, Sodium cyanoborohydride, 9-BBN, IBX, Manganese dioxide, Fetizon reagent, Dioxiranes, Ceric ammonium nitrate, Tebbe reagent, Corey-Nicolaou reagent, Mosher's reagent, use of Os, Ru, and Tl reagents.

Unit 4

15 hours

New synthetic reactions: Baylis-Hillman reaction, Biginelli reaction, Mukaiyama aldol reaction, Mitsunobu reaction, McMurrey reaction, Julia-Lythgoe olefination, and Peterson's stereoselective olefination, Buchwald-Hartwig coupling, Eishenmosher-Tanabe fragmentation and Shapiro reaction, Stork-enamine reaction Aza-Cope, Aza-Wittig reaction, BINAL and BINAP assisted reactions. Ugi reaction, Robinson-Gabriel synthesis, Strecker amino acid synthesis Vilsmeier-Haack reaction, Wohl-Ziegler reaction.

Suggested readings:

1. Finar, I.L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
2. Finar, I.L., (2012). *Organic Chemistry Vol. 2: Stereochemistry and The Chemistry of Natural Products*, Pearson Education, 6th edition, UK.
3. Fleming (1999). *Pericyclic Reactions*, Oxford University Press, Oxford.
4. Fleming (2010). *Molecular Orbitals and Organic Chemical Reactions*, John Wiley & Sons.
5. Jie Jack Li, (2009). *Name Reactions: A collection of Detailed Reaction Mechanism*, Publisher: Springer-verlag
6. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Pub., 3rd edition, New Delhi.
7. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd., New Delhi.
8. Lowry, T.H., Richardson K.S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc.
9. Mc Murry, J., *Organic Chemistry*, Asian Book Pvt Ltd, New Delhi
10. Morrison, R.T., Boyd, R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
11. Mukherjee, S.M., Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
12. Reinhard Bruckner, (2001). *Advanced organic chemistry: Reaction Mechanism*, Academic Press.
13. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
14. Solomn, C.W.G, Fryble, C.B. (2003). *Organic Chemistry*, John Wiley & Sons, Inc., 8th edition, New York.
15. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition, US.
16. W. Carruthers, (2004). *Some Modern Methods of Organic Synthesis*, Cambridge Uni. Press, 4th edition, UK.

Course Title: Bioinorganic Chemistry and Biophysical Chemistry

Paper Code: CMC.556

L	T	P	Cr
4	-	0	4

Learning outcome:

Students who successfully complete this course will be able to

- Understand various aspects of electronic distribution in different energy levels
- Students will understand stereo-chemical aspects of metal complexes and their application in medicinal chemistry
- Understand the phenomenon of reaction kinetics and their applications in medicinal chemistry
- Understand partition coefficient of solutes in different solvent, phenomenon of adsorption and electrochemistry

Unit 1

12 hours

Isomerism; Ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, Magnetic properties of transition metal ions and free ions present, Effects of L-S coupling on magnetic properties, Temperature independent paramagnetism (TIP) in terms of crystal field theory CFT and molecular orbital theory (MOT), Quenching of orbital angular momentum by crystal fields in complexes in terms of splitting. Effect of spin-orbit coupling and A, E & T states mixing, first order and second order Zeeman effects, Spin paired and spin-free equilibria in complexes magnetic properties of polynuclear complexes involving OH, NH₂ and CN bridges.

Unit 2

13 hours

Transition Metal Complexes

Introduction, Potential energy diagram and reactivity of metal complexes, ligand substitution reactions, substitution reactions mechanisms, labile and inert metal complexes, Acid hydrolysis, Factors affecting acid hydrolysis, Base hydrolysis, Conjugate base mechanism, Anation reaction. Substitution reactions in square planar complexes, Trans effect, Mechanism of the substitution reaction Reactions without metal ligand bond cleavage, electron transfer processes outer and inner sphere. The Marcus theory, doubly bridged inner-sphere transfer, other electron transfer reactions; two electron transfers, Non-complementary reaction, Ligand exchange via electron exchange, reductions by hydrated electrons. Applications of metal complexes in Medicinal Chemistry.

Unit 3**11 hours**

Chemical Kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision theory; Potential energy surfaces; transition state theory (statistical and classical treatment); unimolecular reactions and Lindemann mechanism; Solution kinetics factors affecting reaction rate in solution. Effect of solvent and ionic strength (primary salt effect) on the rate constant. Secondary salt effects.

Unit 4**12 hours**

Chemical Equilibrium: Gibbs energy is a minimum with respect to the extent to the extent of reaction, Equilibrium constant is a function of temperature, Standard Gibbs energies of formation is used to calculate Equilibrium constant, Direction of reaction spontaneity, Van't Hoff equation, Molecular partition functions and related thermodynamic data.

Adsorption: Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm: estimation of surface area of solids, Langmuir and Fredulich Isotherms, catalysis.

Unit 5**12 hours**

Electrochemistry: Nernst equation, redox systems, electrochemical cells; electrolytic conductance–Kohlrausch's law and its applications; Fugacity and activity; Activity-coefficients, mean activity coefficients; Debye-Huckel theory (point ion size and finite ion size model); Excess functions; Conductometric and potentiometric titrations.

Nuclear Chemistry: Classification of nuclides, Nuclear stability, Atomic energy, Types of nuclear reactions-fission and fusion, Conservation in nuclear reactions-linear momentum and mass-energy, Reaction cross-section, Bohr's compound nucleus theory of nuclear reaction.

Suggested Books

1. Drago, Russell S. *Physical Methods for Chemists*, 2nd edition, Saunders College Publishing, 1992.
2. Ebsworth, E.A.V.; Rankin, D.W.H.; Cracock, S. *Structural Methods in Inorganic Chemistry*, 1st edition, ELBS, 1987.
3. Cotton, F.A.; Lippard, S.J. *Progress in Inorganic Chemistry*, Vol. 8, Vol. 15, Wiley Internationals.
4. Huheey, James E. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th edition, Harper Collins College Publishers, 1993
5. Glasstone, S. (1951). *Textbook of physical chemistry*.Tata McGraw-Hill, 2007.
6. *Text Book of Physical Chemistry*, K. L. Kapoor, Macmillan, 2006.
7. Tinoco, I., Sauer, K., Wang, J. C., Puglisi, J. D., Harbison, G., & Rovnyak, D. (1995). *Physical chemistry: principles and applications in biological sciences* (Vol. 552, p. 553). Englewood Cliffs, NJ:: Prentice Hall.

8. McQuarrie, D. A. (1997). Physical Chemistry A molecular approach (No. 539 M34).
9. Moore, J. W., & Pearson, R. G. (1961). Kinetics and mechanism. John Wiley & Sons.
10. Glasstone, S. (1951). Textbook of physical chemistry.
11. T. Engel, and P. Reid (2012) Physical Chemistry, Prentice-Hall.

Course Title: Nuclear Chemistry
Paper Code: CMC.557

L	T	P	Cr
4	-	0	4

Learning outcome:

Students who successfully complete this course will be able to

- Understand the nuclear structure and its stability
- Understand nuclear reactions and different fission model
- Know the elements of radiation chemistry

Unit 1

13 hours

Nuclear Structure and Stability

Binding energy, empirical mass equation, nuclear models, the liquid drop model, the shell model, the Fermi gas model & collective nuclear model, nuclear spin, parity & magnetic moments of odd mass numbers nuclei.

Unit 2

17 hours

Nuclear reaction

Introduction, Production of projectiles, nuclear cross section, nuclear dynamics, threshold energy of nuclear reaction, Coulomb scattering, potential barrier, potential well, formation of a compound nucleus, Nuclear reactions, direct Nuclear reactions, heavy ion induced nuclear reactions, photonuclear reactions.

Nuclear fission

Liquid drop model of fission, fission barrier and threshold, fission cross section, mass energy and charge distribution of fission products, symmetric and Asymmetric fission, decay chains and delayed neutrons.

Unit 3

17 hours

Reactor Theory

Nuclear fission as a source of energy, Nuclear chain reacting systems, critical size of a reaction, research reactors, graphite moderated, heterogeneous, enriched uranium reactors, light water moderated, heterogeneous, enriched

uranium reactors, water boilers enriched aq. Homogeneous reactors, Thermonuclear reactors, gamma interactions, shielding and health protection. Reactors in India.

Nuclear Resources in India

Uranium and Thorium resources in India and their extractions, Heavy water manufacturing in India.

Unit 4

13 hours

Elements of Radiation Chemistry

Radiation Chemistry, Interaction of radiation with matter, Passage of neutrons through matter, Interaction of gamma radiation with matter, Units for measuring radiation absorption, Radiolysis of water, Free radicals in water radiolysis, Radiolysis of some aqueous solutions

Suggested readings:

1. Friedlander, G., Kennedy, J. W., & Macias, E. S. (1981). Nuclear and radiochemistry. John Wiley & Sons.
2. Harvey, B. G. (1962). Introduction to Nuclear Physics and Chemistry. Soil Science, 94(4), 274.
3. Haissinsky, M. (1964). Nuclear chemistry and its applications. Addison-Wesley Pub. Co..
5. Choppin, G. R., Liljenzin, J. O., & Rydberg, J. (2002). Radiochemistry and nuclear chemistry. Butterworth-Heinemann.
6. Friedlander, G., Kennedy, J. W., & Macias, E. S. (1981). Nuclear and radiochemistry. John Wiley & Sons.
7. Kanne, W. R. (1961). Basic Principles of Nuclear Science and Reactors. Journal of the American Chemical Society, 83(2), 508-508.
8. Darmstadter, J., Landsberg, H. H., & Morton, H. C. (1983). Energy, today and tomorrow: living with uncertainty. Prentice Hall.
9. Kenneth: Nuclear Power Today, Tomorrow: ELBS
10. Arnikar, H. J. (1995). Essentials of nuclear chemistry (No. 1653). New Age International.
12. Cottingham, W. N., Greenwood, D. A., & Greenwood, D. A. (2001). An introduction to nuclear physics. Cambridge University Press.

Semester-4

Course Title: Organic Chemistry-IV
Paper Code: CMC.571

L	T	P	Cr
4	1	0	4

Learning Outcomes:

Students who successfully complete this course will be able to:

- Understand the asymmetric synthesis, chiral resolution and apply it on the resolution of chiral drugs.
- The basics of organic chemistry will enable understand students to build knowledge in drug synthesis and their interaction with receptors

Unit 1

11 hours

Asymmetric synthesis, chiral pools, chiral catalysis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic, Chemo- regio- and stereoselective transformations, Organocatalysis and biocatalysis

Unit 2

15 hours

Reaction of ylides: Phosphorus ylide; Structure and reactivity, stabilized ylides, effects of ligands on reactivity, Wittig, Wittig-Horner and Wadsworth, Emmons reactions-mechanistic realization; E/Z selectivity for olefin formation, Schlosser modification: Peterson's olefin synthesis. Sulphur Ylides; Stabilized and non-stabilized ylides: Thermodynamically and kinetically controlled reactions with carbonyl compounds, regio- and stereo-selective reactions

Unit 3

17 hours

Alkylation: Enolates: Regio- and stereo-selectivity in enolate generation. "O" versus "C" alkylation, Effect of solvent, Counter cation and Electrophiles; Symbiotic effect; Thermodynamically and kinetically controlled enolate formations; Various transition state models to explain stereoselective enolate formation; Enamines and metallo-enamines; Regioselectivity in generation, Application in controlling the selectivity of alkylation.

Unit 4

17 hours

Protection and deprotection of various functional groups:

Protection of alcohols by ether, silyl ethers and ester formations and their deprotection, Protection of 1, 2 diols- by acetal, ketal and carbonate formation and their deprotection, Protection of amines by acetylation, benzylation,

benzyloxy carbonyl, t-butoxycarbonyl, fmoc, triphenyl methyl groups and their deprotection, Protection of carbonyls by acetal and ketal formation and their deprotection, Protection of carboxylic acids by ester formation and their deprotection

Suggested readings

1. Claydon, J., Gleeves, N., Warren, S., Wothers, P.; (2001) *Organic chemistry*, Oxford University Press, UK.
2. Fieser and Fieser, (2011). *Reagents for organic synthesis, Vol 1-26*. Wiley Interscience, 3rd edition.
3. Finar, I.L., (2012). *Organic Chemistry*, Pearson Education, 6th edition, UK.
4. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
5. Reich, H.J., Rigby, M., (1999). *Handbook of Reagents for Organic Synthesis Acidic and Basic Reagents Vol. IV* Wiley-Interscience
6. Warren, S., (2010). *Organic synthesis: The Synthron Approach*. John Wiley & Sons, New York,
7. Corey E.J., Cheng Xue-Min, (1989) *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons,.
8. Fuhrhop Jürgen, Penzlin Gustav, (1994) *Organic Synthesis: Concepts methods, Starting Materials*, Pubs: Verlagchemie,.
9. Davies Stephen G., (1994) *Organotransition Metal Chemistry: Application to Organic Synthesis*, Pubs: Pergamon Press.
10. Morrison J. D. (1992) (eds) *Asymmetric Synthesis*, Vol. 1 to 5, Pubs: Academic Press.
11. Aitken R.A. and Kilenyi S.N., (1994) *Asymmetric Synthesis*, Pubs: Academic Press..
12. Garry, P. (1996) *Asymmetric Synthesis*, Pubs: Academic Press

Course Title: Green Chemistry

Paper Code: CMC.572

Learning outcome

Students who successfully complete this course will be able to

- Understand various aspects of green chemistry for sustainable development
- Utilize ionic liquids and solid supported reaction conditions to reduce or eliminate use of volatile organic solvents
- Use water as solvent in chemical transformations
- Utilize MW and sonicator in organic synthesis

L	T	P	Cr
3	1	0	4

Unit 1

17 hours

Introduction to green chemistry: History, need and goals. Green chemistry and sustainability, dimensions of sustainability, limitations/obstacles in pursuit of the goals of green chemistry. Opportunities for the next generation of materials designers to create a safer future. Basic principles of green chemistry: Atom economy and scope, Prevention/Minimization of hazardous/toxic products, Designing safer chemicals, Selection of appropriate auxiliary substances (solvents, separation agents etc), use of renewable starting materials, Avoidance of unnecessary derivatization-careful use of blocking/protection groups. Use of catalytic reagents (wherever possible) in preference to stoichiometric reagents, Designing biodegradable products, Prevention of chemical accidents, Strengthening/development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes. Development of accurate and reliable sensors and monitors for real time in process monitoring.

Unit 2

17 hours

Approaches to green synthesis: Basic principles of green synthesis. Different approaches to green synthesis, Use of green reagents in green synthesis: polymer supported reagents, polymer supported peptide coupling reagents. Green catalysts, Phase-transfer catalysts in green synthesis. Advantages of PTC, Reactions to green synthesis, Application of PTCs in C-alkylation, N-alkylation, S-alkylation. Darzens reaction, Williamsons synthesis, Wittig reaction, Click Chemistry. Use of Crown ethers in esterification, saponification, anhydride formation, aromatic substitution and elimination reactions. Ionic liquids as green solvents.

Unit 3

15 hours

Microwave induced and ultrasound assisted green synthesis: Introduction to synthetic organic transformation under microwave (i) Microwave assisted reactions in water (ii) Microwave assisted reactions in organic solvents. (iii) Microwave solvent free reactions Ultrasound assisted reactions: Introduction, substitution reactions, addition, oxidation, reduction reactions. Biocatalysts in organic synthesis: Introduction, Biochemical oxidation and reductions.

Unit 4

11 hours

Organic synthesis in aqueous phase and in solid state: Aqueous reactions. Solid state reactions (i) Solid phase synthesis without using any solvent (ii) Solid supported synthesis.

Suggested Readings:

1. Ahulwalia, V.K.; Kidwai M. (2004). *New Trends in Green Chemistry*, Springer

- Anastas, P.T.; Warner J. C. (2000). *Green chemistry, Theory and Practical*. Oxford University Press.
- Grieco, P.A. (1997). *Organic Synthesis in Water*. Publisher: Kluwer Academic.
- Matlack, A. (2010). *Introduction to green chemistry*. CRC Press.
- Ahluwalia, V. K. (2011). *Green Chemistry: Greener Alternatives to Synthetic Organic Transformations*. Alpha Science International.

Course Title: Medicinal Chemistry-III

L	T	P	Cr
4	0	0	4

Paper Code: CMC.573

Learning outcome: Students who successfully complete this course will be able to

- Understand various biological functions of steroids in the human body
- Understand the role of opioid receptors and role of opioids as analgesic and their abuse potential, psychoactive compounds and their role in neurological disorders
- Explore role of diuretics, cardiovascular agents, antianginals and vasodilators in different disease state
- Understand the role of various antibiotics, antimalarial, antiviral agents and their mechanism of action

Unit 1

15 Hours

Steroids: Introduction, nomenclature, stereochemistry of cholesterol, stigmasterol, ergosterol, diosgenin, solasodine, bile acids, biosynthesis of testosterone, β -estradiol and aldosterone from cholesterol, Estrogens, SAR among estrogens, progestational agents, synthesis of progesterone from diosgenin and stigmasterol, ethisterone from dehydroepiandrosterone, oral contraceptives, SAR of progestins, **Androgens and Anabolic Agents:** Synthesis of testosterone from diosgenin, methyltestosterone from dehydroepiandrosterone, methandienone from methyl testosterone, stanozolol from testosterone. **Aderenocorticoids:** Glucocorticoids and their SAR, mineralocorticoids, modifications in structure of hydrocortisone.

Unit 2

15 Hours

Opioid analgesics: Morphine and related drugs, synthetic modifications of morphine, codeine and thebaine, synthetic analgesics, endogenous opioid peptides, opioid antagonists, **CNS stimulants:** natural and synthetic, Methylxanthines and modified Methylxanthines, Psychopharmacological agents, Antipsychotics, Phenothiazines, **Antidepressants:** Tricyclic

antidepressants, MAO inhibitors, atypical antidepressants, **Antianxiety drugs:** Meprobamate and related drugs, Benzodiazepines, Hallucinogens
Hallucinogenic agents related to indoles, phenethylamines and Cannabinoids.

Unit 3

15 Hours

Diuretics carbonic anhydrase inhibitors: Thiazides and related drugs, High-ceiling diuretics. Aldosterone, antagonists, other potassium sparing diuretics, Osmotic diuretics, **Cardiovascular Agents:** cardiac glycosides, SAR, mechanism of action, toxic effects. Antihypertensive agents; introduction, ganglion blocking agents, antiadrenergic agents, drugs acting directly on smooth muscles, drugs acting on CNS. **Antianginals and vasodilators:** introduction, mechanism of smooth muscle vasodilation, esters of nitrous and nitric acid, side-effects. Antiarrhythmic and antifibrillic drugs classification of antiarrhythmic drugs, mechanism of action, side effects. Angiotensin II receptor antagonists.

Unit 4

15 Hours

Sulphonamides: Introduction and classification, antimicrobial spectrum, DHFR inhibitors, toxicity and side effects, reduction. **Antibiotics:** Classification, cycloserine, chloramphenicol, penicillins, cephalosporins, aminoglycosides, tetracyclines, polypeptides.

Antimycobacterial agents: Introduction, uses in therapeutics. **Antimalarials:** quinoline and analogues, 8-amino quinolines, 9-amino acridines, 4-amino quinolines, diamino pyrimidine, and biguanides and recently introduced compounds. **Antiamoebic agents:** quinoline derivatives, metal free substances, diloxanide furoate, etc. **Anthelmintic drugs** in cestode infections in trematode infections and for intestinal nematode infections, antifilarial agents, **Antiviral agents:** Introduction to DNA, RNA and retroviruses, viral application, amantidine hydrochloride, interferones, acyclovir, idoxuridine, trifluorothymidine and vidarabine etc.

Suggested Readings

1. Delgado, J. N. and Remers W A, Ed. (2010). *Wilson & Gisvold's Textbook of Organic and Pharmaceutical Chemistry*, J. Lippincott Co., 7th edition, Philadelphia.
2. Foye, W. O. (2008). *Principles of Medicinal Chemistry*, Publisher: Lea and Febiger, 6th edition, Philadelphia.
3. King, F. D. (2003). *Medicinal Chemistry Principles and Practice*, Royale Society of Chemistry, 2nd Edition, London.
4. Nogardy, T. and Weaver D F (2005). *Medicinal Chemistry: A Molecular and Biochemical Approach*, Oxford University Press, 3rd edition, New York.

5. Patrick, G.L. (2009). *An Introduction to Medicinal Chemistry*, Oxford University Press, 4th edition. UK.
6. Singh, H., Kapoor, V.K. (Latest Edition). *Medicinal and Pharmaceutical Chemistry* Vallabh Prakashan, Delhi.
7. Smith, H.J. (2006). *Introduction to the Principles of Drug Design and Action*, Taylor and Francis, 4th edition, UK.
8. Wermuth, C.G. (2009). *The Practice of Medicinal Chemistry*, Academic Press (Elsevier), 3rd edition.
9. Wolff, M E, Ed., (2010). *Burger's Medicinal Chemistry and Drug Discovery*, John Wiley and Sons, New York.

Course Title: Organic Chemistry Worksheet-I (DEC-I)

L	T	P	Cr
2	-	-	2

Paper Code: CMC.574

Learning outcome:

Students who successfully complete this course will be able to do:

- IUPAC nomenclature of organic molecules
- Fundamentals of stereochemistry
- Study of reaction intermediates
- Analytical skill development

Unit-1

15 hours

IUPAC nomenclature of organic molecules including regio- and stereoisomers, Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.

Unit-1I

15 hours

Principles of stereochemistry: Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity and asymmetric induction

Unit-1II

15 hours

Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzyne and nitrenes.

Unit-1V

15 hours

Organic reaction mechanisms involving addition, elimination and substitution reactions with electrophilic, nucleophilic or radical species. Determination of reaction pathways.

Suggested Readings:

1. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry Organic Chemistry* Oxford press, 2nd edition
2. Finar, I.L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
3. Mc Murry J., *Organic Chemistry*, Asian Book Pvt. Ltd, 8th edition, New Delhi
4. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
5. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, New Delhi-110002.
6. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age International (P) Ltd., 5th edition, New Delhi.
7. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
8. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., 3rd edition, New Delhi.
9. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
10. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, New York.
11. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
12. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry*. Macmillan India Ltd., 3rd edition, New Delhi.
13. Roberts, J. D., & Caserio, M. C. (1977). *Basic principles of organic chemistry*. WA Benjamin, Inc..
14. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc., 10th edition.
15. Sykes, P. (1986). *A guidebook to mechanism in organic chemistry*. Pearson Education India.
16. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

Course Title: Organic Chemistry Worksheet-II (DEC-II)

L	T	P	Cr
2	-	-	2

Paper Code: CMC.575**Learning outcome**

Students who successfully complete this course will be able to understand:

- Common named reactions and rearrangements
- Concepts in organic synthesis
- Structure determination of organic compounds
- Analytical skill development

Unit-I**15 hours**

Common named reactions and rearrangements – applications in organic synthesis. Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.

Unit-II**15 hours**

Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups. Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.

Unit-III**15 hours**

Pericyclic reactions – electrocycloisatation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry. Synthesis and reactivity of common heterocyclic compounds containing one or two heteroatoms (O, N, S)

Unit-IV**15 hours**

Chemistry of natural products: Carbohydrates, proteins and peptides, fatty acids, nucleic acids, terpenes, steroids and alkaloids. Biogenesis of terpenoids and alkaloids. Structure determination of organic compounds by IR, UV-Vis, ^1H & ^{13}C NMR and Mass spectroscopic techniques.

Suggested readings

1. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3rd edition.
2. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2012). *Organic chemistry* Oxford press, 2nd edition

3. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, India.
4. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
5. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age International (P) Ltd., 5th edition, New Delhi.
6. Bansal, R.K. (2010). *Heterocyclic Chemistry*, New Age International (P) Ltd., 5th edition, New Delhi.
7. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B*, Springer, 5th edition.
8. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
9. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, US.
10. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
11. Joule, J.A., Mills, K. (2010). *Heterocyclic Chemistry*, Blackwell Publishers, 5th edition, New York.
12. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.
15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.
16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistry* Elsevier, 3rd edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, US.
19. Norman, R.O.C.; Coxon, J.M. *Principles of Organic Synthesis*, Blackie Academic & Professional.
20. Warren, S., (2010). *Organic synthesis: The Synthon Approach*. John Wiley & Sons, New York,
21. Warren, S., (2010). *Designing organic synthesis: A Disconnection Approach*. John Wiley & Sons, New York.
22. Corey E.J., Cheng Xue-Min, *The Logic of Chemical Synthesis*, Pubs: John Wiley & Sons, (1989).

23. Silverstein, R. M., Webster, F. X., Kiemle, D. J., & Bryce, D. L. (2014). *Spectrometric identification of organic compounds*. John Wiley & Sons.
24. Skoog, Douglas A. Titulo: *Principles of instrumental analysis* / Douglas A. Skoog, F.
25. James Holler, Timothy A. Nieman. P. imprenta: Madrid, Esp.: McGRAW HILL. *Instrumental methods of analysis* – Willards, 7th edition, CBS publishers.
26. Beckett, A. H., & Stenlake, J. B. (Eds.). (1988). *Practical Pharmaceutical Chemistry: Part II*. Fourth Edition (Vol. 2). A&C Black..
27. Kemp, W. (1991). *Organic spectroscopy* (pp. 42-51). London: Macmillan.
28. Sethi, P. D. (1985). *Quantitative analysis of drugs in pharmaceutical formulations*. Unique Publishers.
29. Munson, J. W. (Ed.). (1984). *Pharmaceutical analysis: modern methods* (Vol. 11). CRC Press.
30. Kalsi, P. S. (2007). *Spectroscopy of organic compounds*. New Age International.
31. Connors, K. A. (2007). *A textbook of pharmaceutical analysis*. John Wiley & Sons.

Course Title: Project
Paper Code: CMC.599

L	T	P	Cr
-	-	-	6

Learning outcome: Students who successfully complete this course will be able to

- Design a research problem and prepare synopsis
- Plan and execute experiments in the laboratory
- Interpret and analyze the results

Evaluation criteria:

- Literature survey/background information
- Organization of content
- Physical presentation
- Questions and answers
- Report evaluation

The following are some of the **modes of classroom transaction**

- | | |
|------------------------------|-----------------------------|
| 1) Lecture | 7) Focused group discussion |
| 2) Demonstration | 8) Team teaching |
| 3) Lecture cum demonstration | 9) Experimentation |
| 4) Project Method | 10) Tutorial |
| 5) Seminar | 11) Problem solving |
| 6) Group discussion | 12) Self-learning |

The following **tools** can be used in **different transactional modes**:

- PPT
- Facebook
- WhatsApp
- Video
- Multimedia packages
- TED Talks
- google drive

Software tools

- Tracker
- Chemdraw
- Schrodinger maestro
- ppt/impress
- Blast
- Endnote

IQAC